Progress In Electromagnetics Research, PIER 48, 279–299, 2004

FAST CONVERGING AND WIDELY APPLICABLE FORMULATION OF THE DIFFERENTIAL THEORY FOR ANISOTROPIC GRATINGS

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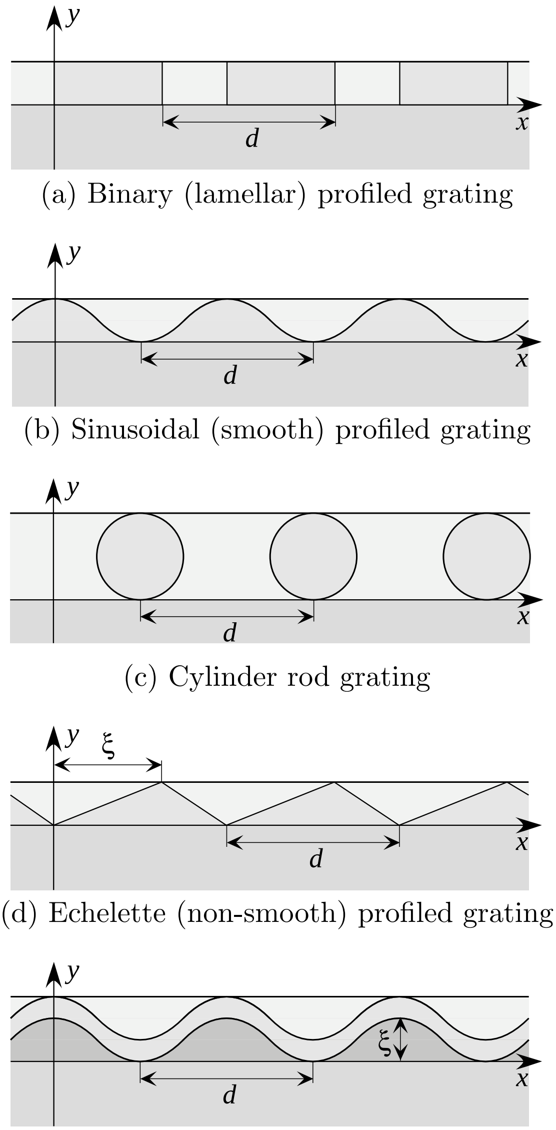
Abstract—The differential method for arbitrary profiled one-dimensional gratings made of anisotropic media is reformulated by taking into account Li's Fourier factorization rules [10] though the present formulation uses the intuitive Laurent rule only. The study concerns arbitrary profiled gratings with both types of electric and magnetic anisotropy, and includes the case of lossy materials. Diffraction efficiencies computed by the present formulation are compared with previous ones, and numerical results show that convergence of the present formulation is superior to the conventional one and comparable convergence with the previous works based on Li's rules.

1. INTRODUCTION

The differential theory [1, 2] is one of the most commonly used approaches in the analyses of various gratings because of its simplicity and wide applicability. The theory introduce a generalized Fourier series expansion, and Maxwell's equations are transformed into a coupled ordinary differential-equation set by using Fourier factorization rules. Outside the groove region, the fields can be expressed in Rayleigh expansions, and thus the solution inside the grating region can be matched to them. Then the diffraction problem is reduced to the numerical integration problem of a coupled differential-equation set with the boundary condition at the top and the bottom of the grating layer. The differential method in narrow sense (DM) transforms this problem into an initial-value problem through the shooting method[2] and then solved with the help of numerical integration algorithms. Besides there is a widely used variant of the theory called the rigorous coupled-wave method (RCWM) [3–5], which introduces a staircase approximation and each grating profile is represented by several layers of lamellar gratings. The coefficients of the coupled differential-equation set are constant in each layer, and then the problem can be solved by eigensystem analysis.

Various types of gratings are shown in Fig. 1 and they can be analyzed using the differential theory when the gratings are shallow or made of nonconducting materials. However, numerical experiments for deep gratings with large truncation order show in many cases numerical instabilities occur. Trouble comes from the accumulation of contamination linked with growing exponential functions. A simple way to get rid of this problem is to use the scattering-matrix (S-matrix) propagation algorithm [6–8]. Also, a difficulty concerning to the convergence was criticized for deep gratings made of conducting materials[9] and this approach was thought to be limited in its application range during about 30 years. The origin of poor convergence was explained by Li's Fourier factorization rules [10], which gave an idea for accelerating the convergence. Li proposed RCWM formulations for isotropic[10] and anisotropic[11] gratings made of conducting materials by taking into account the rules. RCWM is well suited for lamellar profiled gratings shown as Fig. 1(a) but recent papers [12, 8] showed the staircase approximation used on RCWM was doubtful about its efficiency for arbitrary profiled gratings made of conducting materials. Popov and Nevière [13] investigated the TM diffraction problem on arbitrary profiled gratings made of isotropic materials and presented DM formulations based on Li's Fourier factorization rules. Watanabe et al. [14, 15] introduced continuous intermediary functions and proposed a DM formulation for smooth profiled gratings (Fig. 1(b)) made of anisotropic materials. Popov and Nevière [16] formally generalized this approach to the scattering problems on arbitrary profiled periodic surface that is assumed to have normal vector everywhere and separates two anisotropic



(a) Binary (lamellar) profiled grating

(b) Sinusoidal (smooth) profiled grating

(c) Cylinder rod grating

(d) Echelette (non-smooth) profiled grating

(e) Multi-layered grating

Figure 1. Various types of gratings.

media. However, their idea seems not to be easy to apply individual problems, and also they gave no numerical experiment of anisotropic grating. Also, cylindrical rod gratings (Fig. 1(c)) made of anisotropic materials are formulated in Ref. [17]. Watanabe [18] presented another approach for nonsmooth profiled gratings (Fig. 1(d)) made of anisotropic materials with the use of discontinuous intermediary functions. One of the remained profiles important in engineering is a multi-layered grating as shown in Fig. 1(e). Metallic gratings are sometimes coated with one or more dielectric layers to prevent the grating surface from tarnishing or to enhance diffraction efficiency [19].

This paper generalizes the formulation given in Ref. [17] and proposes a DM formulation that is applicable to all the one-dimensional gratings shown in Fig. 1. The study concerns both types of electric and magnetic anisotropy and includes the case of lossy materials. Also, it concerns conical diffraction problem, in which the incident plane is not parallel to the direction of grating periodicity. The formulation uses the continuous intermediary functions introduced in Refs. [14, 15] and Li's Fourier factorize rules are applied to derive the constitutive relations in Fourier space. As mentioned above, there have been many formulations based on Li's Fourier factorization rules [10, 11, 13–18]. However, all of them have been proposed for individual types of gratings and limited their application ranges. Also, the Fourier coefficients of the grating profile functions are required to derive the coupled differential-equation set, but their analytical expressions are rarely obtained and a long computation time is necessary for numerical integration in many problems. The present formulation covers all the gratings in Fig. 1 and gets rid of the processes of numerical integrations for arbitrary profiled gratings. Numerical experiments show a great advantage of the present formulation compared with the conventional one, in which the Laurent rule is used for Fourier factorization without any care of the continuity properties, and comparable convergence with the previous works based on Li's rules.

2. STATEMENT OF THE PROBLEM

We shall investigate the diffraction problem on gratings made of anisotropic materials. Figure 2 shows an example of geometry under consideration. We consider time harmonic fields assuming a time-dependence in $e^{-i\omega t}$, and deal with the plane incident wave propagating in the direction of polar angle θ ($0 \le \theta < \pi/2$) and azimuth angle ϕ ($-\pi < \phi \le \pi$). The grating structure is uniform in the z-direction, and the x-axis is parallel to the direction of periodicity. The grating depth is denoted by h and, the relative permittivity and

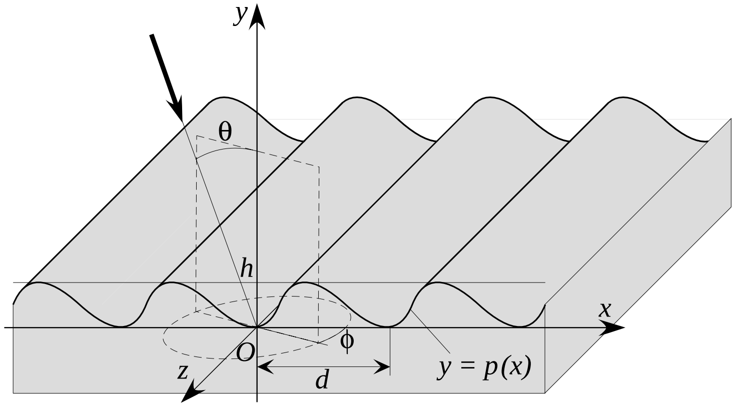


Figure 2. Geometry of a grating under consideration.

the relative permeability are given by $\overline{\overline{\boldsymbol{\varepsilon}}}(x, y)$ and $\overline{\overline{\boldsymbol{\mu}}}(x, y)$ that are periodic in the x-direction with the period d. Inside the grating layer $0 \leq y \leq h$, the electromagnetic parameters $\overline{\overline{\boldsymbol{\varepsilon}}}(x, y)$ and $\overline{\overline{\boldsymbol{\mu}}}(x, y)$ are supposed to be piecewise constant functions of x for each y, and have L discontinuous boundaries in a periodicity cell though the number L may be depend on y. As shown in Fig. 3, the equations of these discontinuous boundaries are denoted by $x = g_j(y)$ $(j = 1, \cdots, L)$ in such a way that $0 < g_1(y) < \cdots < g_L(y) \leq d$, and we put $g_0(y) = g_L(y) - d$ for the sake of convenience. The (p, q)-entries $(p, q = x, y, z)$ of the relative permittivity and the relative permeability matrices are constant in $g_{j-1}(y) < x < g_j(y)$ $(j = 1, \cdots, L)$ and the values are $\varepsilon_{j,pq}$ and $\mu_{j,pq}$, respectively. Also, the angles between the tangent at $x = g_j(y)$ and the x-angle are denoted by $\eta_j(y)$. The cover region $y > h$ is filled with a lossless, homogeneous, and isotropic material described by the relative permittivity ε_c and the relative permeability μ_c, and a homogeneous and anisotropic material which fills the substrate region $y < 0$ is described by a relative permittivity matrix $\overline{\overline{\boldsymbol{\varepsilon}}}_s$ and $\overline{\overline{\boldsymbol{\mu}}}_s$. Throughout the paper, we normalize the fields, namely the E-field by $\sqrt[4]{\mu_0/\varepsilon_0}$, the H-field by $\sqrt[4]{\varepsilon_0/\mu_0}$, the D-field by $\varepsilon_0 \sqrt[4]{\mu_0/\varepsilon_0}$, and the B-field by $\mu_0 \sqrt[4]{\varepsilon_0/\mu_0}$, where ε_0 and μ_0 denote the permittivity and the permeability in free space, respectively.

The Floquet theorem claims that the Cartesian components of the fields are pseudo-periodic when the structure is periodic. Therefore all the components can be approximately expressed by truncated generalized Fourier series; for example the x component of E-field can

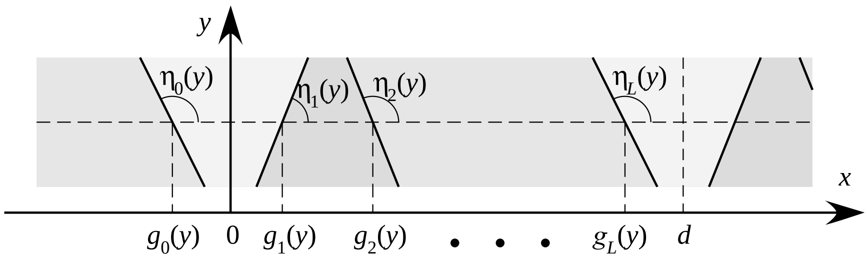


Figure 3. Discontinuous boundaries inside the grating layer.

be written as

$$E_x(x,y,z) = \sum_{n=-N}^{N} E_{x,n}(y)\, e^{i\,k_0(\alpha_n\,x+\gamma\,z)} \tag{1}$$

with

$$\alpha_n = \sqrt{\varepsilon_c\,\mu_c}\,\sin\theta\,\cos\phi + n\,\frac{\lambda_0}{d} \tag{2}$$

$$\gamma = \sqrt{\varepsilon_c\,\mu_c}\,\sin\theta\,\sin\phi \tag{3}$$

where N is the truncation order, λ_0 is the wavelength in free space, and $E_{x,n}(y)$ are the nth-order generalized Fourier coefficients that are functions of y only. To treat the generalized Fourier coefficients systematically, we introduce column matrices; for example the coefficients of E_x are expressed by a column matrix $[E_x]$ that is defined by

$$[E_x] = \left(E_{x,-N} \quad \cdots \quad E_{x,N}\right)^t, \tag{4}$$

where the superscript t denotes the transpose matrix. The coefficients of other field components are expressed in the same way.

All the periodic and pseudo-periodic functions in Maxwell's curl equations are replaced with their Fourier series and the constitutive relations in the Fourier space, which express the relations between the generalized Fourier coefficients of E, H-fields and D, B-fields, are given. Then, as shown by Popov and Nevière[16], we may obtain the following coupled differential-equation set:

$$\frac{d}{dy}\,\boldsymbol{f}(y) = i\,k_0\,\boldsymbol{M}(y)\,\boldsymbol{f}(y) \tag{5}$$

with

$$\boldsymbol{f}(y) = \begin{pmatrix} [E_x] \\ [E_z] \\ [H_x] \\ [H_z] \end{pmatrix} \tag{6}$$

where the expression of $(8N+4) \times (8N+4)$ square matrix $\boldsymbol{M}(y)$ is given in Refs. [16, 18].

As mentioned before, the electromagnetic fields outside the grating layer can be expressed in Rayleigh expansions, and then the problem is reduced to the problem of a coupled differential-equation set with boundary conditions at the top and the bottom of the grating layer. In order to apply the S-matrix propagation algorithm, the grating layer is decomposed into several or more sublayers. Then the transmission matrices of each sublayer, which are obtained by usual numerical integration schemes, built up the S-matrix for entire grating structure. We calculate the transmission matrices by using the two-stage fourth-order implicit Runge-Kutta scheme based on Gauss-Legendre quadrature because Ref. [8] pointed out that implicit integration schemes provide stable calculations.

3. CONSTITUTIVE RELATIONS IN FOURIER SPACE

The important point for fast converging formulation is that the expression of the constitutive relations in the Fourier space is constructed by following Li's Fourier factorization rules. The constitutive relations in the original space are written as follows:

$$\begin{pmatrix} D_x \\ D_y \\ D_z \end{pmatrix} = \sum_{m=1}^{L} w_m \begin{pmatrix} \varepsilon_{m,xx} & \varepsilon_{m,xy} & \varepsilon_{m,xz} \\ \varepsilon_{m,yx} & \varepsilon_{m,yy} & \varepsilon_{m,yz} \\ \varepsilon_{m,zx} & \varepsilon_{m,zy} & \varepsilon_{m,zz} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} \tag{7}$$

$$\begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix} = \sum_{m=1}^{L} w_m \begin{pmatrix} \mu_{m,xx} & \mu_{m,xy} & \mu_{m,xz} \\ \mu_{m,yx} & \mu_{m,yy} & \mu_{m,yz} \\ \mu_{m,zx} & \mu_{m,zy} & \mu_{m,zz} \end{pmatrix} \begin{pmatrix} H_x \\ H_y \\ H_z \end{pmatrix} \tag{8}$$

These relations are transformed into the truncated Fourier space and expressed as follows:

$$\begin{pmatrix} [D_x] \\ [D_y] \\ [D_z] \end{pmatrix} = \sum_{m=1}^{L} \boldsymbol{C}_m^{(e)} \begin{pmatrix} [w_m\, E_x] \\ [w_m\, E_y] \\ [w_m\, E_z] \end{pmatrix} \tag{9}$$

$$\begin{pmatrix}[B_x]\\ [B_y]\\ [B_z]\end{pmatrix} = \sum_{m=1}^{L} \boldsymbol{C}_m^{(h)} \begin{pmatrix}[w_m\, H_x]\\ [w_m\, H_y]\\ [w_m\, H_z]\end{pmatrix} \tag{10}$$

with

$$\boldsymbol{C}_m^{(e)} = \begin{pmatrix}\varepsilon_{m,xx}\,\boldsymbol{I} & \varepsilon_{m,xy}\,\boldsymbol{I} & \varepsilon_{m,xz}\,\boldsymbol{I}\\ \varepsilon_{m,yx}\,\boldsymbol{I} & \varepsilon_{m,yy}\,\boldsymbol{I} & \varepsilon_{m,yz}\,\boldsymbol{I}\\ \varepsilon_{m,zx}\,\boldsymbol{I} & \varepsilon_{m,zy}\,\boldsymbol{I} & \varepsilon_{m,zz}\,\boldsymbol{I}\end{pmatrix} \tag{11}$$

$$\boldsymbol{C}_m^{(h)} = \begin{pmatrix}\mu_{m,xx}\,\boldsymbol{I} & \mu_{m,xy}\,\boldsymbol{I} & \mu_{m,xz}\,\boldsymbol{I}\\ \mu_{m,yx}\,\boldsymbol{I} & \mu_{m,yy}\,\boldsymbol{I} & \mu_{m,yz}\,\boldsymbol{I}\\ \mu_{m,zx}\,\boldsymbol{I} & \mu_{m,zy}\,\boldsymbol{I} & \mu_{m,zz}\,\boldsymbol{I}\end{pmatrix} \tag{12}$$

where $\boldsymbol{I}$ denotes the identity matrix. In order to derive the constitutive relation in the Fourier space, we need to factorize the Fourier coefficients of the products of w_m and the electromagnetic field components. Li [10] pointed out that the Laurent rule is valid only for a product of two periodic functions that have no concurrent jump discontinuities (type 1 product in Li's terminology), and another Fourier factorization rule named the inverse rule can be adopted, in many case, to a product of two functions that have only pairwise-complementary jump discontinuities (type 2 product). However, a product of two functions have concurrent but not complementary jump discontinuities (type 3 product) can be Fourier factorized by neither the Laurent nor the inverse rules. As a conclusion, we have to derive the constitutive relations in the Fourier space by using type 1 and type 2 products only. Also, since the inverse rule is noticed to be a consequence of the Laurent rule [14], we try to present a formulation leading to type 1 products only.

Here, we consider two continuous functions $s(x,y)$ and $c(x,y)$ that are $s_j(y) = \sin[\eta_j(y)]$ and $c_j(y) = \cos[\eta_j(y)]$ on the boundaries $x = g_j(y)$ and appropriately interpolated between the boundaries. The linear interpolation is used in this paper and they are given in $g_{j-1}(y) < x < g_j(y)$ as follows:

$$s(x,y) = \frac{s_j - s_{j-1}}{g_j - g_{j-1}}\, x + \frac{g_j\, s_{j-1} - g_{j-1}\, s_j}{g_j - g_{j-1}} \tag{13}$$

$$c(x,y) = \frac{c_j - c_{j-1}}{g_j - g_{j-1}}\, x + \frac{g_j\, c_{j-1} - c_{j-1}\, s_j}{g_j - g_{j-1}}. \tag{14}$$

However, we should note that $s(x,y)$ and $c(x,y)$ must be defined so as not to vanish simultaneously for any x. This condition is required for the inversion calculation appeared later in Eq. (46).

Now, we introduce the intermediary functions D_n, E_t, B_n, and H_t, which are defined by the functions $s(x,z)$ and $c(x,z)$ as follows:

$$\begin{pmatrix} D_n \\ E_t \end{pmatrix} = \sum_{m=1}^{L} w_m \begin{pmatrix} t^{(e)}_{m,nx} & t^{(e)}_{m,ny} & t^{(e)}_{m,nz} \\ c & s & 0 \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} \tag{15}$$

$$\begin{pmatrix} B_n \\ H_t \end{pmatrix} = \sum_{m=1}^{L} w_m \begin{pmatrix} t^{(h)}_{m,nx} & t^{(h)}_{m,ny} & t^{(h)}_{m,nz} \\ c & s & 0 \end{pmatrix} \begin{pmatrix} H_x \\ H_y \\ H_z \end{pmatrix} \tag{16}$$

with

$$t^{(e)}_{m,np}(x,y) = -\varepsilon_{m,xp}\, s(x,y) + \varepsilon_{m,yp}\, c(x,y) \tag{17}$$

$$t^{(h)}_{m,np}(x,y) = -\mu_{m,xp}\, s(x,y) + \mu_{m,yp}\, c(x,y). \tag{18}$$

These four functions have no physical meaning but, on the boundaries $x = g_j(y)$, D_n, B_n give the normal components of D, B-fields, and E_t, H_t give the tangential component of E, H-fields. Hence, they are continuous functions of x for each y because of the laws of electromagnetism, and pseudo-periodic in the x-direction like the field components.

Multiplying equations (15) and (16) by w_l, and using the relations: $w_l\, w_m = \delta_{l,m}\, w_l$, we obtain

$$w_l \begin{pmatrix} D_n \\ E_t \end{pmatrix} = w_l \begin{pmatrix} t^{(e)}_{l,nx} & t^{(e)}_{l,ny} & t^{(e)}_{l,nz} \\ c & s & 0 \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} \tag{19}$$

$$w_l \begin{pmatrix} B_n \\ H_t \end{pmatrix} = w_l \begin{pmatrix} t^{(h)}_{l,nx} & t^{(h)}_{l,ny} & t^{(h)}_{l,nz} \\ c & s & 0 \end{pmatrix} \begin{pmatrix} H_x \\ H_y \\ H_z \end{pmatrix}. \tag{20}$$

Then, after inversion calculation, we get

$$w_l \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} = w_l \begin{pmatrix} a^{(e)}_{l,xn} & a^{(e)}_{l,xt} & a^{(e)}_{l,xz} \\ a^{(e)}_{l,yn} & a^{(e)}_{l,yt} & a^{(e)}_{l,yz} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} D_n \\ E_t \\ E_z \end{pmatrix} \tag{21}$$

$$w_l \begin{pmatrix} H_x \\ H_y \\ H_z \end{pmatrix} = w_l \begin{pmatrix} a^{(h)}_{l,xn} & a^{(h)}_{l,xt} & a^{(h)}_{l,xz} \\ a^{(h)}_{l,yn} & a^{(h)}_{l,yt} & a^{(h)}_{l,yz} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} B_n \\ H_t \\ H_z \end{pmatrix} \tag{22}$$

with

$$a_{l,xn}^{(e)} = -s/\xi_l^{(e)} \tag{23}$$
$$a_{l,xt}^{(e)} = -\left(\varepsilon_{l,xy}\, s - \varepsilon_{l,yy}\, c\right)/\xi_l^{(e)} \tag{24}$$
$$a_{l,xz}^{(e)} = -\left(\varepsilon_{l,xz}\, s - \varepsilon_{l,yz}\, c\right) s/\xi_l^{(e)} \tag{25}$$
$$a_{l,yn}^{(e)} = c/\xi_l^{(e)} \tag{26}$$
$$a_{l,yt}^{(e)} = \left(\varepsilon_{l,xx}\, s - \varepsilon_{l,yx}\, c\right)/\xi_l^{(e)} \tag{27}$$
$$a_{l,yz}^{(e)} = \left(\varepsilon_{l,xz}\, s - \varepsilon_{l,yz}\, c\right) c/\xi_l^{(e)} \tag{28}$$
$$a_{l,xn}^{(h)} = -s/\xi_l^{(h)} \tag{29}$$
$$a_{l,xt}^{(h)} = -\left(\mu_{l,xy}\, s - \mu_{l,yy}\, c\right)/\xi_l^{(h)} \tag{30}$$
$$a_{l,xz}^{(h)} = -\left(\mu_{l,xz}\, s - \mu_{l,yz}\, c\right) s/\xi_l^{(h)} \tag{31}$$
$$a_{l,yn}^{(h)} = c/\xi_l^{(h)} \tag{32}$$
$$a_{l,yt}^{(h)} = \left(\mu_{l,xx}\, s - \mu_{l,yx}\, c\right)/\xi_l^{(h)} \tag{33}$$
$$a_{l,yz}^{(h)} = \left(\mu_{l,xz}\, s - \mu_{l,yz}\, c\right) c/\xi_l^{(h)} \tag{34}$$
$$\xi_l^{(e)} = \varepsilon_{l,xx}\, s^2 - \left(\varepsilon_{l,xy} + \varepsilon_{l,yx}\right) s\, c + \varepsilon_{l,yy}\, c^2 \tag{35}$$
$$\xi_l^{(h)} = \mu_{l,xx}\, s^2 - \left(\mu_{l,xy} + \mu_{l,yx}\right) s\, c + \mu_{l,yy}\, c^2. \tag{36}$$

Since D_n, E_t, E_z, B_n, H_t, H_z and the functions given by Eqs. (23)–(34) are continuous everywhere, all terms on the right-had sides in Eqs. (21) and (22) are type 1 products. Consequently, Eqs. (21) and (22) are transformed into the Fourier space with careful use of the Laurent rule, and we obtain the following relations:

$$\begin{pmatrix} [w_l\, E_x] \\ [w_l\, E_y] \\ [w_l\, E_z] \end{pmatrix} = \boldsymbol{A}_l^{(e)} \begin{pmatrix} [D_n] \\ [E_t] \\ [E_z] \end{pmatrix} \tag{37}$$

$$\begin{pmatrix} [w_l\, H_x] \\ [w_l\, H_y] \\ [w_l\, H_z] \end{pmatrix} = \boldsymbol{A}_l^{(h)} \begin{pmatrix} [B_n] \\ [H_t] \\ [H_z] \end{pmatrix} \tag{38}$$

with

$$\boldsymbol{A}_l^{(f)} = \begin{pmatrix} [\![w_l]\!]\,[\![a_{l,xn}^{(f)}]\!] & [\![w_l]\!]\,[\![a_{l,xt}^{(f)}]\!] & [\![w_l]\!]\,[\![a_{l,xz}^{(f)}]\!] \\ [\![w_l]\!]\,[\![a_{l,yn}^{(f)}]\!] & [\![w_l]\!]\,[\![a_{l,yt}^{(f)}]\!] & [\![w_l]\!]\,[\![a_{l,yz}^{(f)}]\!] \\ \boldsymbol{0} & \boldsymbol{0} & [\![w_l]\!] \end{pmatrix} \tag{39}$$

for $f = e, h$. Considering the relations: $\sum_{l=1}^{L} w_l = 1$, we can derive the relations between the generalized Fourier coefficients of the electromagnetic fields components and the intermediary functions as follows:

$$\begin{pmatrix} [E_x] \\ [E_y] \\ [E_z] \end{pmatrix} = \sum_{l=1}^{L} \boldsymbol{A}_l^{(e)} \begin{pmatrix} [D_n] \\ [E_t] \\ [E_z] \end{pmatrix} \tag{40}$$

$$\begin{pmatrix} [H_x] \\ [H_y] \\ [H_z] \end{pmatrix} = \sum_{l=1}^{L} \boldsymbol{A}_l^{(h)} \begin{pmatrix} [B_n] \\ [H_t] \\ [H_z] \end{pmatrix}. \tag{41}$$

These equations are substituted into Eqs. (37) and (38), and we have

$$\begin{pmatrix} [w_m\, E_x] \\ [w_m\, E_y] \\ [w_m\, E_z] \end{pmatrix} = \boldsymbol{A}_m^{(e)} \left(\sum_{l=1}^{L} \boldsymbol{A}_l^{(e)} \right)^{-1} \begin{pmatrix} [E_x] \\ [E_y] \\ [E_z] \end{pmatrix} \tag{42}$$

$$\begin{pmatrix} [w_m\, H_x] \\ [w_m\, H_y] \\ [w_m\, H_z] \end{pmatrix} = \boldsymbol{A}_m^{(h)} \left(\sum_{l=1}^{L} \boldsymbol{A}_l^{(h)} \right)^{-1} \begin{pmatrix} [H_x] \\ [H_y] \\ [H_z] \end{pmatrix}. \tag{43}$$

Then, from Eqs. (9) and (10), the constitutive relations in the Fourier space can be derived in the following form:

$$\begin{pmatrix} [D_x] \\ [D_y] \\ [D_z] \end{pmatrix} = \boldsymbol{Q}^{(e)} \begin{pmatrix} [E_x] \\ [E_y] \\ [E_z] \end{pmatrix} \tag{44}$$

$$\begin{pmatrix} [B_x] \\ [B_y] \\ [B_z] \end{pmatrix} = \boldsymbol{Q}^{(h)} \begin{pmatrix} [H_x] \\ [H_y] \\ [H_z] \end{pmatrix} \tag{45}$$

with

$$\boldsymbol{Q}^{(f)} = \left(\sum_{m=1}^{L} \boldsymbol{C}_m^{(f)}\, \boldsymbol{A}_m^{(f)} \right) \left(\sum_{l=1}^{L} \boldsymbol{A}_l^{(f)} \right)^{-1} \tag{46}$$

for $f = e, h$. The coupled differential-equation set (5) is derived by using the obtained relations (44)–(46).

4. COMPARISON WITH PREVIOUS WORKS

In order to validate the proposed formulation, we consider below specific examples and show some numerical results concerning the diffraction efficiencies of gratings made of anisotropic and conducting materials. On numerical calculation, a TM polarized (the H-field is perpendicular to the y-axis) plane incident wave with $\theta = 30^\circ$, $\phi = 20^\circ$, and the wavelength in free space $\lambda_0 = 0.6328\,\mu\text{m}$ is always used. Cobalt is chosen as the anisotropic material, in which the Cartesian components of the relative permittivity matrix are $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = -8.19 + i\,16.38$, $\varepsilon_{xz} = -\varepsilon_{zx} = -0.495 - i\,0.106$, $\varepsilon_{xy} = \varepsilon_{yx} = \varepsilon_{yz} = \varepsilon_{zy} = 0$ and the relative permeability is given by the identity matrix. Also, 50 steps (5 layers in the S-matrix propagation algorithm and 10 steps per layer) with equal thickness are used to integrate the coupled-equation set. This step number is large enough to give precise integration when the grating depth is less than the wavelength in free space [8]. The obtained results are compared with the conventional formulation [20], in which the coefficient matrices $\boldsymbol{Q}^{(f)}$ $(f = e, h)$ appeared in Eqs. (44) and (45) are given by

$$\boldsymbol{Q}^{(f)} = \sum_{m=1}^{L} \boldsymbol{C}_m^{(f)} \begin{pmatrix} [\![w_m]\!] & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & [\![w_m]\!] & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & [\![w_m]\!] \end{pmatrix}. \tag{47}$$

The Fourier coefficients of $a_{l,pq}^{(f)}$ $(f = e, h;\ l = 1, \cdots, L;\ p = x, y, z;$ and $q = n, t, z)$ defined by Eqs. (23)–(34) are required to calculate the coefficient matrix of the coupled differential-equation set (5) for each y. However their explicit expressions are unknown in many problems and long computation time is necessary for numerical integration. To reduce the computation time, the coefficients of $a_{l,pq}^{(f)}$ are calculated from those of $s(x, y)$ and $c(x, y)$ with the use of the approximation formulas given in Appendix A of Ref. [15]. Note that several equivalent expressions can be obtained depending on how we apply the approximation formulas on the various products. In this paper, we omit these long and tedious expressions, but the author confirms the convergence speed is almost independent of these equivalent expressions and is ready to provide the used expressions to any interested reader.

First, we consider lamellar profiled gratings, which include binary gratings shown in Fig. 1(a) and stacks of binary gratings. In this case, the discontinuous boundaries for each y in the grating layer are perpendicular to the x-axis. Therefore, if we set $\eta_j(y) = \pi/2$ for all j and use the approximation formulas, the present formulation is equivalent to the formulation in Ref. [14]. The present formulation is also shown to be equivalent to the formulation in Ref. [11] when the permeability is assumed to be a constant μ_0 everywhere. These formulations proposed in Refs. [11, 15] are numerically validated by a strong improvement of the convergence speed compared with that for the conventional formulation (47).

Next, we consider smooth profiled gratings including sinusoidal profiled gratings shown in Fig. 1(b). Supposing that the equation of the discontinuous boundary inside the grating layer is given by $y = p(x)$, $p(x)$ is a known periodic and continuous function that with a continuous derivative. References [14, 15] were devoted to them and got fast converging formulations, which is almost equivalent with the present formulation but uses

$$s(x) = \frac{p'(x)}{\sqrt{1 + \{p'(x)\}^2}} \tag{48}$$

$$c(x) = \frac{1}{\sqrt{1 + \{p'(x)\}^2}} \tag{49}$$

instead of the functions $s(x, y)$ and $c(x, y)$ given in Eqs. (13) and (14) on the present formulation. In these equations, $p'(x)$ is the derivative of $p(x)$. Figure 4 shows the efficiencies of -1st and 0th-order diffraction waves computed by three formulations for a sinusoidal profiled bare grating as functions of the truncation order N, which truncates the Fourier series expansion from $-N$th to Nth order. The grating parameters are chosen as follows: $d = 0.6\,\mu\text{m}$, $h = 0.5\,\mu\text{m}$, $p(x) = (h/2)\,[1 + \cos(2\,\pi\,x/d)]$, and the region $y > p(x)$ is free space and the region $y < p(x)$ is filled with the anisotropic material. Then, the number of discontinuous boundaries for each y inside the grating layer is $L = 2$, and the calculations use the following functions:

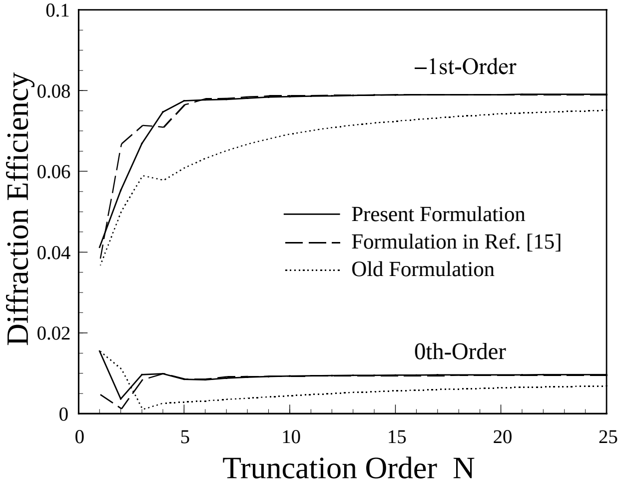
$$g_1(y) = \frac{d}{2\,\pi} \arccos\left(\frac{2}{h}\,y - 1\right) \tag{50}$$

$$g_2(y) = d - g_1(y) \tag{51}$$

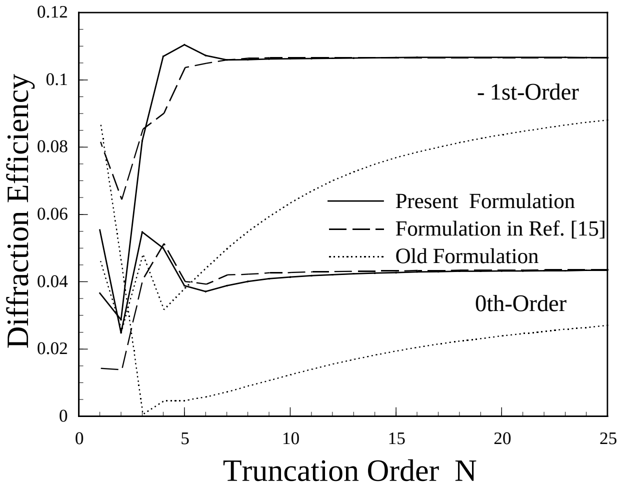
$$\eta_1(y) = -\arctan\left(\frac{2\,\pi\,\sqrt{y\,(h-y)}}{d}\right) \tag{52}$$

$$\eta_2(y) = -\eta_1(y). \tag{53}$$

The solid curves are the results of the present formulation, the dotted curves are those of the conventional formulation, and the dashed curves are those of Ref. [15]'s formulation. The convergence speeds of the



(a) TE diffraction waves



(b) TM diffraction waves

Figure 4. Comparison of convergences of diffraction efficiencies computed by the present, Ref.[15]'s, and the conventional formulations for a sinusoidal grating.

present and Ref. [15]'s formulations, which are both based on Li's Fourier factorization rules, are similar, and superior to that of the conventional formulation. On the formulation in Ref. [15], since $s(x)$ and $c(x)$ given in Eqs. (48) and (49) are independent of y, the Fourier coefficients are calculated once for entire integration process. Hence, Ref. [15]'s formulation costs the shortest computation time to obtain the required precision. However, explicit expressions of the Fourier coefficients of the functions $s(x)$ and $c(x)$ are rarely known for arbitrary profiled gratings and numerical integrations that consume computation time are required in many problems. When the explicit expressions cannot be derived, the computation time of the present formulation becomes comparable with that of Ref. [15] formulation.

For cylinder rod gratings shown in Fig. 1(c), the present formulation becomes same with the formulation published separately in Ref. [17]. Let a be the radius of circular cylinder, and the grating depth becomes $h = 2\,a$ and the discontinuous boundaries are given by the following functions:

$$g_1(y) = \sqrt{y\,(2\,a - y)} \tag{54}$$

$$g_2(y) = d - g_1(y). \tag{55}$$

The tangential angle at the boundary $x = g_1(y)$ can be written as

$$\eta_1(y) = \frac{\pi}{2} - \arctan\frac{a - y}{g_1(y)}. \tag{56}$$

We should note that the numerical calculation fails if the tangential angle on the boundary $x = g_2(y)$ is set in such a way $\eta_2(y) = -\eta_1(y)$. Because $|\eta_1(a) - \eta_2(a)| = \pi$ and, as mentioned before, $s(x, y)$ and $c(x, y)$ defined in Eqs. (13) and (14) vanish simultaneously at the middle point of the boundaries for $y = a$. Consequently, we have to care about the expression of $\eta_2(y)$. One choice of the expression is given as

$$\eta_2(y) = \begin{cases} -\eta_1(y) & \text{for } \frac{a}{2} < |y - a| < a \\ \pi - \eta_1(y) & \text{for } |y - a| \le \frac{a}{2} \end{cases}. \tag{57}$$

Here, we do not show numerical experiments because there are some results of numerical examples in Ref. [17].

Non-smooth profiled gratings including echelette profiled gratings shown in Fig. 1(d) are formulated in Ref. [18] by taking into account Li's Fourier factorization rules. The intermediary functions used in Ref. [18] are discontinuous though they are continuous on the discontinuous boundaries of the electromagnetic parameters. Using the notation ξ

illustrated in Fig. 1(d), the discontinuous boundaries are given by the following functions:

$$g_1(y) = \frac{\xi}{h}\,y \tag{58}$$

$$g_2(y) = -\frac{d-\xi}{h}\,y + d \tag{59}$$

and then the tangential angle at the boundaries can be written as $\eta_1(y) = \arctan(h/\xi)$, $\eta_2(y) = -\arctan(h/(d-\xi))$. Figure 5 provides convergences of the diffraction efficiencies computed by several formulations. The cover region $y > h$ and the region $g_2(y) - d < x < g_1(y)$ are free space, and the substrate region $y < 0$ and the region $g_1(y) < x < g_2(y)$ are filled with the anisotropic material. The grating parameters are chosen as follows: $d = 0.6\,\mu$m, $h = 0.5\,\mu$m, and $\xi = 0.4\,\mu$m. The solid and the dashed curves, which are calculated by the formulations based on Li's Fourier factorization rules, are comparable and provide significant improvements of the convergence compared with the dotted curves calculated by the conventional formulation.

Finally, we show a numerical example of multi-layered grating. We assume that the grating profile is characterized by two sinusoidal equations: $y = p_1(x) = (\xi/2)\,[1 + \cos(2\,\pi\,x/d)]$ and $y = p_2(x) = (\xi/2)\,[1 + \cos(2\,\pi\,x/d)] + h - \xi$ where the notation ξ is defined in Fig. 1(e). The region $y > p_2(x)$ is free space, the region $p_1(x) < y < p_2(x)$ is filled with the anisotropic material, and the region $y < p_1(x)$ is filled with an isotropic and homogeneous material, for which the relative permittivity and permeability are supposed to be 1.55^2 and 1, respectively. Supposing $\xi > h/2$, the number of discontinuous boundaries inside the grating layer is depend on y, namely, $L = 2$ for $0 < y < h - \xi$ and $\xi < y < h$, and $L = 4$ for $h - \xi < y < \xi$. The discontinuous boundaries and the tangential angles are given for $0 < y < h - \xi$:

$$g_1(y) = \frac{d}{2\,\pi}\,\arccos\left(\frac{2}{\xi}\,y - 1\right) \tag{60}$$

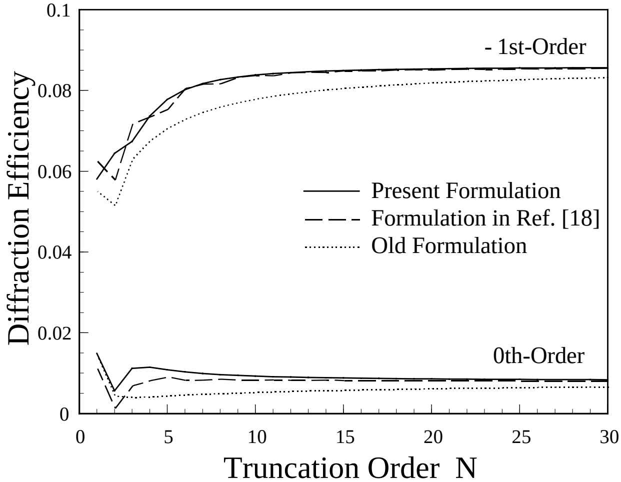
$$g_2(y) = d - g_1(y) \tag{61}$$

$$\eta_1(y) = -\arctan\left\{\frac{2\,\pi\,\sqrt{y\,(\xi - y)}}{d}\right\} \tag{62}$$

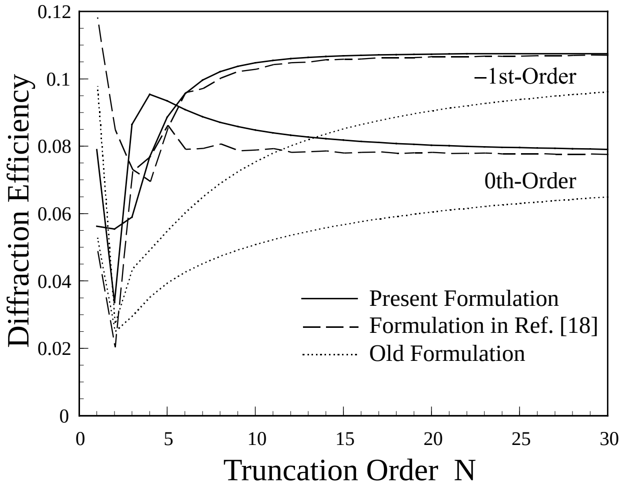
$$\eta_2(y) = -\eta_1(y), \tag{63}$$

for $h - \xi < y < \xi$:

$$g_1(y) = \frac{d}{2\,\pi}\,\arccos\left(\frac{2}{\xi}\,y - 1\right) \tag{64}$$

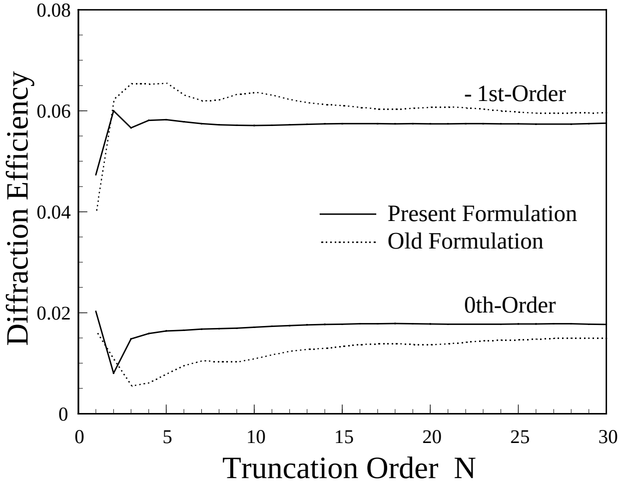


(a) TE diffraction waves

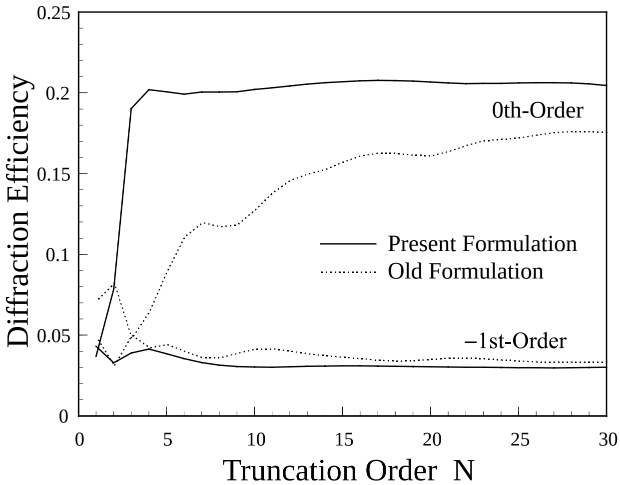


(b) TM diffraction waves

Figure 5. Comparison of convergences of diffraction efficiencies computed by the present, Ref. [18]'s, and the conventional formulations for a echelette grating.



(a) TE diffraction waves



(b) TM diffraction waves

Figure 6. Comparison of convergences of diffraction efficiencies computed by the present and the conventional formulations for a multi-layered grating.

$$g_2(y) = \frac{d}{2\pi}\arccos\left\{\frac{2}{\xi}(y-h+\xi)-1\right\} \tag{65}$$

$$g_3(y) = d - g_2(y) \tag{66}$$

$$g_4(y) = d - g_1(y) \tag{67}$$

$$\eta_1(y) = -\arctan\left\{\frac{2\pi\sqrt{y(\xi-y)}}{d}\right\} \tag{68}$$

$$\eta_2(y) = -\arctan\left\{\frac{2\pi\sqrt{(y-h+\xi)(h-y)}}{d}\right\} \tag{69}$$

$$\eta_3(y) = -\eta_2(y) \tag{70}$$

$$\eta_4(y) = -\eta_1(y), \tag{71}$$

and for $\xi < y < h$:

$$g_1(y) = \frac{d}{2\pi}\arccos\left\{\frac{2}{\xi}(y-h+\xi)-1\right\} \tag{72}$$

$$g_2(y) = d - g_1(y) \tag{73}$$

$$\eta_1(y) = -\arctan\left\{\frac{2\pi\sqrt{(y-h+\xi)(h-y)}}{d}\right\} \tag{74}$$

$$\eta_2(y) = -\eta_1(y). \tag{75}$$

Figure 6 shows the convergences of the present and the conventional formulation by using the following parameters: $d = 0.6\,\mu$m, $h = 0.5\,\mu$m, and $\xi = 0.4\,\mu$m. It is observed that the present formulation provides a significant improvement of convergence.

5. CONCLUSION

This paper presented a fast converging and widely applicable formulation of the differential theory for arbitrary profiled one-dimensional gratings made of anisotropic materials. The formulation is based on Li's Fourier factorization rules [10] though this approach gets rid of the use of the inverse rule and uses the Laurent rule only. The aim of this paper is to show that it can be used successfully for a large class of anisotropic gratings. In this paper, the prescriptive gratings are chosen as numerical examples, but the reader will understand that the application to a lot of other profiles is straightforward without the use of numerical integration. Also, we have supposed that the electromagnetic parameters between the discontinuous boundaries are constant but there is no doubt that extensions to more complicated profiles with inhomogeneous materials could be also done at the cost of some additional work.

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